

Claims

1. A hybrid learning system for searching an experimental space, comprising:

a data mart configured to acquire, store and manipulate at least, historical experimental data, descriptor data, and concurrent experimental data;

5 a search engine configured to use selection techniques to select a set of evaluation points representing a corresponding set of experiments to be run, based on the data from the data mart; and

a point evaluation mechanism configured with

(i) learning modules which perform predictive processing on the

10 evaluation points selected by the search engine, and

(ii) a scoring module which performs a rating operation on outputs of the learning modules to rate the outputs of the learning modules,

15 wherein operation of the data mart, search engine and point evaluation mechanism are operated a plurality of times such that a repeating process is undertaken to obtain a finalized output.

2. The system according to claim 1 further including a physical experiment, wherein results of the physical experiment are supplied to the data mart.

20 3. The system according to claim 2 wherein the experimental space is a Combinatorial Chemistry experimental space.

25 4. The system according to claim 3 wherein an input to the system are experiments and the output of the system is a set of elements that yield a highest turnover number (TON) and selectivity.

5. A method for exploring an experimental space using a hybrid learning system, the method comprising:

- (a) generating an experimental space including a plurality of experimental points, representing potential solutions to an experiment;
- (b) collecting historical experimental data, descriptor data, and concurrent experimental data;
- 5 (c) storing the historical experimental data, descriptor data, and concurrent experimental data in a data mart, wherein the data mart includes the ability to be queried;
- 10 (d) performing a genetic algorithm processing loop on the experimental space to obtain a subset of experimental points from the plurality of experimental points;
- 15 (e) performing a clustering processing loop on the experimental space to obtain a subset of experimental points from the plurality of experimental points;
- (f) selecting the subset of experimental points from at least one of the genetic algorithm processing step and the clustering processing step;
- 20 (g) supplying the selected experimental points and a subset of the data from the data mart to a point evaluation mechanism;
- (h) performing a supervised learning process on the selected points; and
- (i) obtaining an output.

6. The method of claim 5 further including performing a physical experiment using experimental points from the experimental space to obtain actual physical experimental results.

25 7. The method of claim 6 wherein the physical experimental results are supplied to the data mart.

8. The method according to claim 5 wherein steps (b) – (i) are repeated.

9. The method according to claim 5 wherein the experimental space is a Combinatorial Chemistry experimental space.

10. The method of claim 5 wherein the clustering loop includes:

5 (a) partitioning the experimental space into clusters of points having similarities;

(b) selecting a sample from each cluster, the sample being at least one evaluation point, wherein the selected samples are a first generation of evaluation points;

10 (c) performing at least one of actual physical experiments or synthetic models of experiments using the first generation of evaluation points;

(d) scoring each cluster based on an outcome of the at least actual experiment and synthetic models;

(e) selecting a cluster based on the scoring;

15 (f) repartitioning the experimental space into clusters on a reduced space; and

(g) repeating steps (b) – (f).

11. The method of claim 5 wherein genetic algorithm loop includes:

20 (a) partitioning the experimental space into uniform spaces of points;

(b) selecting a sample from each uniform space, the sample being at least one evaluation point, wherein the selected samples are a first generation of evaluation points;

25 (c) performing at least one of actual physical experiments or synthetic models of experiments using the first generation of evaluation points;

(d) scoring each uniform space based on an outcome of the at least actual experiment and synthetic models;

(e) selecting points to be parents based on the scoring;

30 (f) generating a next generation of points based on selected parents; and

(g) repeating steps (b) – (f).

12. The method according to claim 5 wherein each time a set of experiments is performed, additional data is added to the system and a further refined 5 model is generated.

13. The method according to claim 5 wherein the selection processes are run against a new improved model.

10 14. A hybrid learning system for searching an experimental space comprising:

a data mart configured to receive, store and supply data;

15 a search engine including at least a genetic algorithm processor and a clustering processor configured to operate in parallel, both the genetic algorithm processor and the clustering processor configured to request data from the data mart, in order to select a set of points from the experimental space, the points representing a corresponding set of experiments to be undertaken; and

20 a point evaluation mechanism including at least one learning module and a scoring module, the at least one learning module receiving data from the data mart and the search engine and having a model experiment to which the selected points and data are applied.